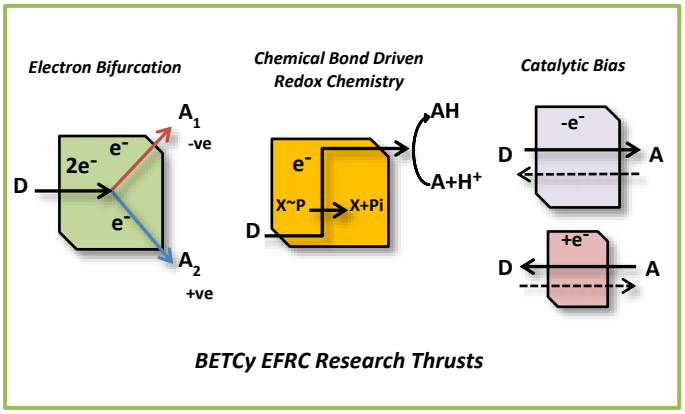
Center for Biological Electron Transfer and Catalysis (*BETCy*)
EFRC Director: John Peters
Lead Institution: Montana State University
Start Date: August 2014

***Mission Statement**: To investigate electron bifurcation, electron-ion coupling, and redox catalysis in model enzymes to provide a detailed understanding of mechanisms of electron transfer reactions involved in the efficient conversion of electrochemical potential into chemical bond energy.*

The focus of the Biological Electron Transfer and Catalysis (*BETCy*) EFRC research is elucidating mechanisms of conversion of electrochemical potential into chemical bond energy and is organized into three integrated Thrusts.

- **Thrust 1** focuses on the mechanism of coupling exergonic and endergonic electron transfer reactions by electron bifurcation.
- **Thrust 2** investigates coupling chemical bond energy and electrochemical potential in electron transfer to achieve very low potential reductions.
- **Thrust 3** focuses on elucidating atomic level determinants of enzymatic redox properties and their relationship to catalytic bias.



BETCy EFRC Research Thrusts

We are developing a collective knowledge of metalloenzymes as models for redox reactions by applying physical science and computational tools to characterize biochemical reactions catalyzed by multi-subunit enzymes harboring arrays of iron-sulfur clusters and flavin cofactors. Understanding these mechanisms is central to overcoming the thermodynamic barriers that currently limit production of reduced products and fuels.

Biological systems have elegant strategies for converting electrochemical potential energy into chemical bond energy (e.g., C-H, H-H, and N-H) stored in reduced compounds that can serve as advanced biofuels. One significant limitation for the production of highly reduced compounds is that their production in natural and industrial processes relies on low oxidation-reduction potential chemicals as feedstocks. However, unique biochemical strategies exist to generate pools of reducing equivalents that can serve as a source of electrons for chemical bond formation from low oxidation-reduction potential feedstocks.

We are focusing on a newly discovered biochemical mechanism termed “electron bifurcation”, which upgrades electrochemical potential by effectively coupling endergonic and exergonic reactions in an overall thermodynamically favorable process. The underlying mechanistic details governing electron bifurcation are, however, still poorly understood and a more in-depth understanding of this phenomenon could lead to “game changing” and transformational advances in strategies to direct electron flow. These studies provide a blueprint for bio-inspired, multi-electron catalytic processes that can ultimately utilize electrons of varying reduction potentials to drive chemical reactions. We are also working to elucidate how biology uses a combination of chemical bond energy and electrochemical potential to accomplish

very difficult reduction of low potential reactions (e.g., CO_2 and N_2 reduction) using electron donors of modest reduction potentials.

The goal of the BETCy EFRC is to provide a fundamental understanding of mechanisms to overcome key thermodynamic barriers that limit the production of reduced products where energy is stored in the form of C-H, H-H, and N-H bonds. The three interrelated research Thrusts of the BETCy EFRC emphasize: mechanisms of electron bifurcation in driving low potential oxidation-reduction reactions. The research of the BETCy EFRC builds on recent seminal discoveries in biology and provides the basis for attacking key knowledge gaps and expanding the knowledge base that is essential for realizing the true potential of bioenergy and bio-inspired catalysis as prominent components of the global energy production portfolio. We have assembled a strong team of investigators with complementary research interests and technical skills to accomplish the proposed interdisciplinary tasks. The work is having a profound scientific impact on understanding and predicting matter and energy at the atomic level and in generating a blueprint for efficient control of electron flow into energy products and chemicals.

The work is directly in line with and addresses three of the five Basic Energy Sciences Advisory Committee (BESAC) Grand Challenges including: *1. Control of material processes at the level of electrons, 2. Design and perfect atom and energy efficient synthesis of revolutionary new forms of matter with tailored properties, 3. Characterize and control matter away, far away, from equilibrium* (which is the essence of electron bifurcation reactions). In addition, the proposed BETCy EFRC goals embrace the Basic Research Needs (BRNs) outlined in the BES Workshop Report on *Catalysis for Energy*, and makes strong connections with the *Hydrogen Economy* and *Solar Energy Utilization* BRNs.

The research plan of the *BETCy* EFRC is designed to exploit unique biochemical mechanisms that have yet to be explored substantively in the context of bioenergy, but that have the potential for innovative advancement. The successful outcome of this research will be a collection of fundamental principles that serve as a blueprint to enable the tailored re-design of biological systems and enzymes to control matter and energy at the level of electrons and molecules to provide the foundations to create new energy technologies.

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